TITLE: Process Modelling of the Fabrication of Critical Rotating Components for Gas Turbine Applications

Process Modelling of the Fabrication of Critical Rotating Components for Gas Turbine Applications

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Abstract

The fabrication of rotating components for a gas turbine engine requires a number of different manufacturing processes: casting, thermal-mechanical shaping (from ingot or powder), heat-treatment, machining and joining. Numerical algorithms and advanced computer hardware/software are being used increasingly to simulate these manufacturing processes and the materials behaviour resulting from them that controls the service performance. The purpose of this paper is to provide the reader with a flavour of the range of research that is being carried out, the benefits that it confers and its current limitations. Finally, some challenges for the future are identified.

1. Introduction

The fabrication of critical rotating components for the hot sections of gas turbine engines, from premium grades of nickel-base superalloys that have been designed specifically for their excellent mechanical behaviour at elevated temperatures, requires a number of different manufacturing processes. These include melting and investment casting, thermal-mechanical working (including forging and rolling), heat treatment, machining and welding (see Fig. 1). The manufacturing stream is complex and normally involves a number of specialist suppliers. Among the characteristics of the manufacturing cycle are: (i) the period required for processing and hence delivery can take many months and involve international transport between various stages, (ii) these delays tie up capital with obvious costs which can be exacerbated by material losses, (iii) the complexity of the manufacturing process can lead to fragmentation and loss of data certifying the quality of material and its susceptibility to performance-limiting defects, and (iv) there is a barrier to responding quickly to changes in specification and the requirements of the end-users, i.e. the gas turbine manufacturers.

Computer modelling is currently being used for the simulation of different stages of the manufacturing process in an effort to deal with these difficulties. In fact the accuracy, speed and sophistication of the computation are improving to such an extent that very significant benefits are now being derived. In the present paper, a number of case studies will be presented which are representative of the UK's state-of-the-art in this field, termed *process modelling*. In the past decade or so, progress has been made at coupling treatments of the *macroscopic* characteristics of the processes to the response of the material on the *microstructural* scale. This is an important stage in relating the process to eventual service

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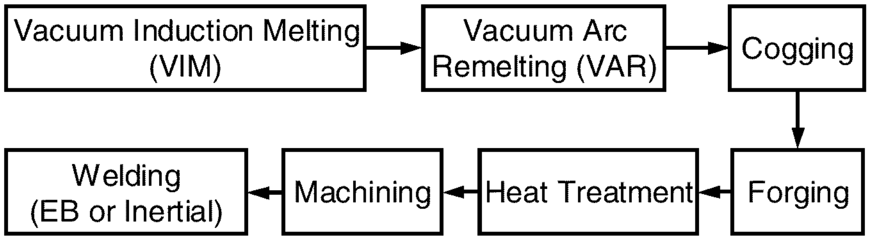

Fig. 1. The manufacturing processes used for the fabrication of turbine discs arrangements.

performance. An important characteristic of the UK process modelling has been extensive collaboration with the gas turbine manufacturers and materials suppliers, who have provided access to manufacturing facilities on the factory floor; these have been instrumented for targeted trials designed to test and calibrate the models. In the final part of the paper some challenges for the future are identified.

2. Background

In order to appreciate the value of process modelling in this context, it is helpful to consider some of the processes in a little detail. Consider first a ‘secondary’ melting process such as vacuum arc remelting (VAR). Its main purposes are to improve the chemical homogeneity of the ingot by eliminating the gross segregation, which is inherited from ‘primary’ vacuum induction melting (VIM), and to produce a sound defect-free ingot for subsequent thermal-mechanical processing. The aim of the modeller will be to help the manufacturing engineer to achieve this homogeneity and material soundness by control of the process variables under his control. In practice, the modeller will make predictions of: (i) the location of the fusion boundary, and any alteration to its location due to changes in processing conditions, (ii) the fraction of the billet that is not subject to steady-state or stationary conditions, (iii) the typical average microstructure that results from the process and (iv) the likely occurrence and stability of defects such as *white spot* or *freckles*, which occur when pieces of the electrode remain unmelted after entering the molten pool or there are convectional instabilities in the melt. Computer modelling represents a very powerful tool for the analysis of these effects.

The use of process modelling for the simulation of the subsequent thermal-mechanical shaping processes can also be contemplated. A typical VAR ingot needs to be worked repeatedly in a ‘cogging’ press in order to refine the as-cast grain structure through repeated sequences of recrystallisation and deformation, which have the further effect of reducing microsegregation. An accurate treatment of these phenomena is the challenge to the modeller. Predictions of the rate of recrystallisation are potentially valuable, so that excessive cost is not incurred due to unnecessary stages in the process. Closed-die forging operations are also amenable to modelling; predictions which might be required include the manner in which the die cavity is filled, so that the deformation sequences can be designed in an optimal fashion, and so that the susceptibility to forging defects can be assessed. Finally, an elastic-plastic analysis of the heat treatment of the blank turbine disc forging is necessary, since residual stresses result from the significant thermal stresses which originate from the quenching operation. These must be known so that any subsequent machining sequences can be chosen appropriately.

Finally, there are examples of assembly processes such as joining, which are highly amenable to modelling and simulation. Consider for example the high-pressure (HP) compressor sections of the aeroengine, which are now often manufactured from superalloys, since the operating conditions are beyond the temperature capability of titanium alloys. The assemblies require joining, often by electron beam welding. Process simulations are useful for the prediction of weld-induced distortions which can sometimes be so large that they exceed the pre-defined tolerances, leading to excessive non-conformance and scrap. Higher strength superalloys are joined by inertia welding, and here significant advantages have been gained through the use of modelling for the optimisation of tooling and jigging arrangements.

In the past, there has been a tendency to treat each stage of the process cycle in isolation. However, the major challenge now facing researchers and industry is to address the complete manufacturing chain to produce compatible and interacting models that can optimise the production of critical components, both in terms of quality and cost. To this end, a multi-institutional initiative is under way in the UK, within the EPSRC's *Materials Processing for Engineering Applications (MAPEA)* initiative, to develop and validate models for turbine disc manufacture. The aim is to track the structure, including possible defects, from the initial cast ingot to the final product in order to minimise unnecessary scrap in late stage of the manufacture.

3. Process Modelling of Manufacturing Processes

It is beyond the scope of this paper to give a rigorous analysis of all of the various approaches to process modelling. Rather, we give some examples of recent developments and of work in progress to illustrate the progress that is being made.

3.1 Solidification Processing

Nickel-base alloys are often produced by a combination of primary and secondary remelting processes followed by thermal mechanical processing or an investment casting operation to produce varying complexity of rotating parts. Control of structure and avoidance of defects in both process routes requires a detailed understanding of the solidification processes. Modelling of these processes can help predict both the average structure, the deviation about this average, and can give insight into the conditions causing defects (both intrinsic and extrinsic) which often limit the performance of the material in service.

VACUUM ARC REMELTING

VAR is one of the principal secondary-melting technologies used to produce nickel-base superalloys for the manufacture of turbine-discs in aero-engines. It operates on either a *Vacuum Induction Melted* (VIM) ingot or VIM barstock that has been *Electro Slag Refined* (ESR) to remove unwanted inclusions. VAR is used to produce a sound ingot that is free of macroscopic segregation and has a relatively fine and homogeneous grain structure. An arc is struck between the starting ingot (VAR or VAR/ESR) and a water-cooled crucible; the ingot progressively melts and drips into the crucible where it solidifies in a controlled manner. The intense heat in the arc and melt pool helps to further reduce the number of inclusions. However, a number of types of defect that can be generated in the VAR process and be carried through to later process stages. These include *inclusions* that originate from ceramics used in VIM processing, *white spot* that is associated with fall-in from the electrode or alloy skull (illustrated schematically in Fig. 2) and *freckles* that are localised macrosegregate caused by convection instabilities. A numerical model is being developed to simulate the VAR process that allows the process control parameters and alloy properties to be related to the formation of a range of microstructural features and defects. This will help enable the processing conditions for new alloys to be optimised with a minimum of time-consuming trial and error experimentation.

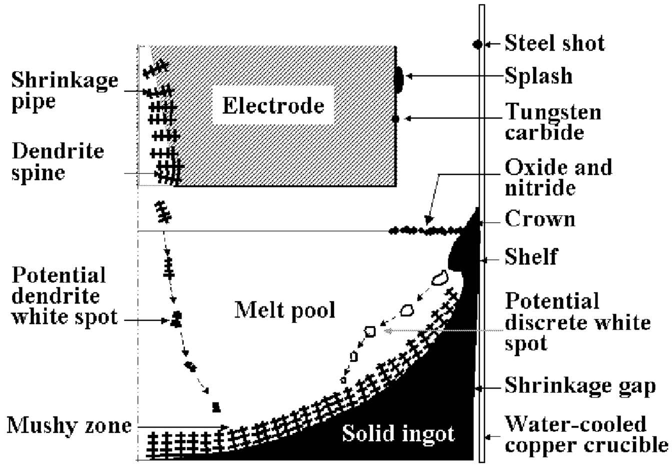

Fig. 2. Schematic of the potential origins of white spots in VAR.

A multiscale model was developed to simulate the VAR process, with different spatial and temporal modelling scales being used depending on the problem being addressed. The fluid flow and heat transport in the melt pool and mushy zone of ingot are described by the incompressible form of the Navier-Stokes equations and the accompanying energy and electromagnetic conservation equations. These equations are solved simultaneously using an in-house transient finite volume model with a moving mesh. This allows the influence of even small process perturbations to be studied at almost any stage of the process. Fig. 3a shows the predicted flow field for one set of conditions, whilst Fig. 4a shows both the flow and thermal fields near the melt pool when the ingot has reached half its final length for typical conditions. Validation of the model is ongoing against instrumented trials on both laboratory scale and using an industrial VAR furnace.

One important application of the model has been the prediction of inclusion survival. Fig. 2 schematically illustrates the most common sources of intrinsic and extrinsic inclusions, including: various types of *white spot* (a zone lean in niobium), splash, and the extrinsic defects such as tungsten carbide and steel shot. White spot can arise from dendrites in the shrinkage pipe of the VIM electrode or from the first solid fraction that forms as the shelf or skull in contact with the water-cooled mould falling through the molten pool and being entrapped in the mushy zone before completely melting. If the solid debris is melted or dissolved in the VAR molten pool then it is likely to be innocuous. If it falls to the bottom of the pool and is incorporated in the semi-solid region, it can either survive as a foreign inclusion or as a white spot compositional heterogeneity.

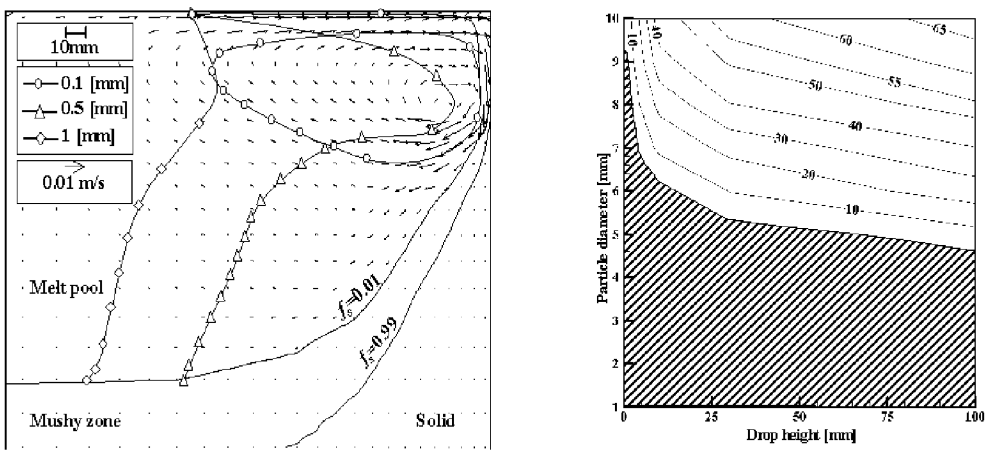

Fig. 3. (a) Simulated fall-in trajectories for three initial spherical particles sizes. (b) Process map illustrating the remaining volume percentage of a dendrite-cluster as a function of drop height H, shaded area is white spot free.

The consequences of various types of solid-matter falling into the VAR melt pool have been considered. Simulations of particle cluster trajectory, temperature distributions and dissolution were performed for alloy and process parameters relevant to industrial VAR processing of INCONEL 718 (Fig. 3a).[1, 2] Operational safety windows for the avoidance of white spot were plotted as a function of the cluster size and composition for each variable. The drop height, composition and the initial particle temperature all had a significant influence on the potential for white spot formation. However, the operational safety window was most sensitive to the composition and drop height. Process maps were produced to indicate the potential for white spot formation as a function of the principal process variables and particle characteristics. Fig. 3b shows the importance of the drop height of dendrite fall-in on the dissolution rate. Such maps offer the potential to tailor the process conditions to specific alloys in order to avoid the formation of detrimental white spot.

The model was also used to determine which types of extraneous particles, such as steel shot, tungsten carbide tool tips, etc, have the potential to pass through the molten pool without completely remelting, producing an inclusion in the final ingot.[2] Steel shot particles were found to present little risk of forming inclusions in the VAR process. The similar densities of steel and superalloy lead to long residence times in the melt; a melting time of 1.5 seconds for the largest particle considered indicates that a steel shot particle will not be able to reach the mushy zone before dissolving. Tungsten carbide particles, however, have little buoyancy in the superalloy melt and rapidly drop to the semi-solid region, presenting a high risk of forming detrimental inclusions. This model was used to reduce VAR costs by determining when shot peening was not required between melts.

The thermal and fluid flow conditions in the melt have a profound effect on the microstructures produced in the solid ingot; this in turn determines the subsequent behaviour during forging and in service. One objective of the multiscale models has been to predict the development of grain structure throughout the entire processing chain, including VAR processing. The thermal profiles as a function of time generated by the macromodel were passed to a mesoscale model to predict the different microstructural features. This mesomodel is a cellular automata (CA) model, that tracks not only the average grain sizes and their distributions, but also their morphology and texture indicating; for example, the conditions leading to a transition from columnar to equiaxed grain growth. The predicted grain structure is compared to the experimentally observed structure in Fig. 4. The model also predicts how strong of a perturbation in processing conditions is required to produce areas of discontinuous grain morphology (and hence how tightly the process must be controlled). One such discontinuity is termed a *tree ring* structure, and has been linked to the onset of freckle. Tree rings are zones of fine equiaxed grains interrupting the continuity of the columnar grain structure that predominates over the outer half of VAR ingots. The model also predicts these discontinuities, as shown by the highlighted squares in Fig. 4b&c. The duration and magnitude of perturbations required to form heterogeneities in the grain structure was systematically investigated, allowing process windows to be determined for the prevention of these defects.[3]

In summary, the combination of experiments at the industrial and laboratory scale and the development of a multi-scale model have provided detailed insight into the VAR process. This potentially provides a process optimisation tool that can reduce the expensive and time-consuming commissioning of VAR processing of new alloys. By linking mesoscopic models to the continuum VAR model, key features that limit the final performance can be predicted, including grain development (such as tree-rings) and the dissolution/melting of exogenous particles in the melt pool. This has allowed the production of process maps that link the occurrence of tree-rings and white spot to the major process variables. Application of these maps to prevent defects has a massive financial impact, especially for defects that may not be detected until further downstream in the process.

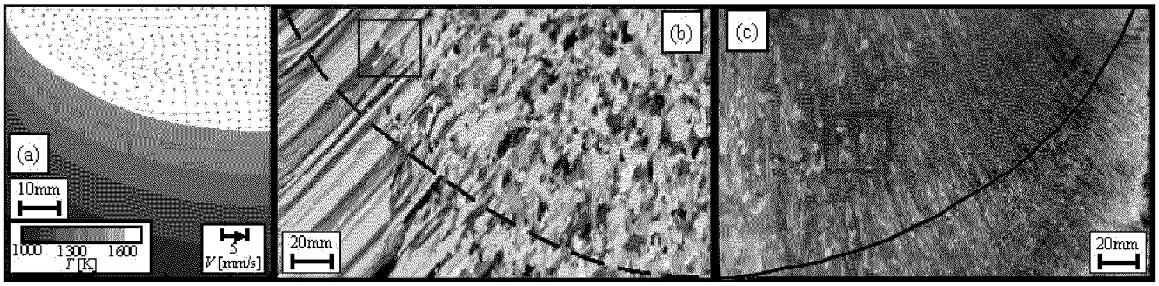

Fig. 4. (a) Macromodel predicted temperatures and fluid flow near the melt pool. Comparison of (b) multiscale model predicted and (c) experimentally observed (optical macrograph) grain structure. The melt pool shape is shown as a black line, predicted by the macromodel in (b) and calculated from the tree rings in (c).

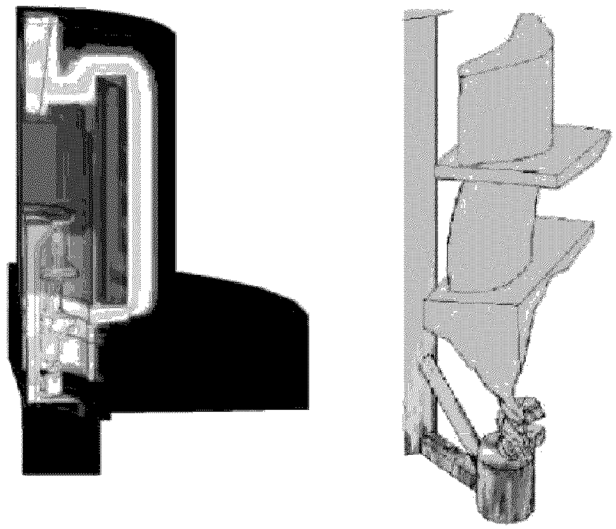

Fig. 5. Process model of the investment casting of high pressure turbine blading. (a) Thermal model. (b) Predicted grain structure.

3.2 Investment Casting

Process simulations of the investment casting of directionally solidified and single crystal turbine blade aerofoils are now also possible[4], as indicated in Fig. 5. Heat transfer during solidification of shaped castings in furnaces with complex baffle-geometry can be calculated using appropriate radiation factors to allow the shape of the mushy zone, the temperature gradients and the rate of solidification to be estimated with some precision. The heat transfer analyses have been coupled with grain structure calculations based upon the cellular automata technique, such that stochastic calculations of grain density can be made. The analyses are suitable for the evaluation of novel designs of grain selector, and also the evaluation of the susceptibility to stray grain formation around re-entrant features such as shrouds. These kinds of computational tools have been used to identify the optimal processing conditions required for the production of new types of turbine blade, with significant savings in costs and time via reductions in the number of design/make iterations. In a typical foundry, the probability of any given casting being defective is significant; modelling represents a powerful tool for dealing with this situation. Indeed, it is claimed by one industrial concern with which the authors have worked that costs running into many millions of pounds have been saved.

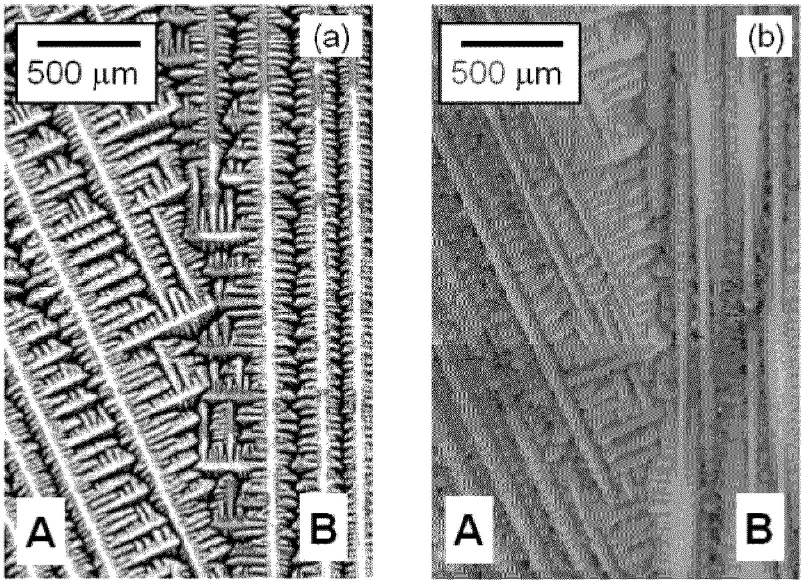

Fig. 6 (a) Predicted and (b) experimental results (after ref. 2) of competitive growth for two diverging grains, A and B, with misorientations of 25° and 1°, respectively.

The effectiveness of numerical models requires that they incorporate an appropriate knowledge of the physics controlling the process under consideration. The characteristic range of orientations produced and the propensity to stray grain formation in single crystal castings varies very significantly between alloys with small compositional differences. The modelling techniques are now being extended to include full tracking of the solute profiles at the micron scale and simulation of the dendritic morphologies. This allows the competition between dendrites growing at an arbitrary angle of misorientation to be simulated. Due to the increase in tip undercooling, for constrained growth in a constant thermal gradient, dendrites with a preferred growth direction will grow faster than those that are misoriented, with the preferred orientations overgrowing misoriented ones. This effect was shown experimentally by Wagner *et al.*[5] for two bicrystals crystals of CMSX4 superalloy grown with different misorientations, one with converging and the other with diverging dendrites. The experimental conditions of Wagner *et al.*[5] were simulated using a cellular automata-finite difference (CA-FD) model two grains of 1° and 25° misorientation grown in divergent directions (see Fig. 6(a)). The highly misoriented grain must form ternary dendrite arms to maintain its growth in the direction of the gradient, showing excellent qualitative agreement to the experiments of Wagner *et al* (Fig. 6(b)). The challenge is to understand why alloys with marginal differences in chemistry behave so differently and to define the process conditions required for optimum single crystal processing.

3.3 Simulation of Thermal-Mechanical Working and Heat Treatment

During the manufacture of high integrity superalloy disc components for gas turbines, the forgemaster carries out a series of forging operations to shape a pre-forged billet to within as near the required component shape as possible, in order to minimise costs associated with machining and excessive waste of material. Most usually, stringent limits will be placed on the grain size induced by processing; this is to ensure adequate mechanical properties and a capability for non-destructive testing (NDT). In practice, successful processing requires the optimum amount of deformation to be imposed at the correct temperature within the right time-scale. The relationships between the processing parameters, the flow-field and the metallurgical structure are time dependent and strongly temperature dependent. Historically, great reliance has been placed on the skill and experience of the forgemaster to determine optimum processing conditions.

Nowadays, finite-element (FEM) based models are being used routinely to enable forging procedures to be designed and analysed before resorting to trials on the factory floor, see Fig. 7. However, before the simulations can be made, it is necessary to quantify the rheological behaviour of the material using laboratory-scale compression tests and to carry out data reduction to determine the appropriate mechanical and structural constitutive equations, which are usually viscoplastic in nature.[6] Within the computer these manifest themselves as datasets which are read by the software and materials subroutines which estimate the evolution of metallurgical structure, i.e. the fraction of grains recrystallised, grain size.[7] In practice, the simulations prove very useful for (i) estimating whether the load capacity of the press is likely to be exceeded, usually at the latter stages of processing (ii) the evolution of the temperature field, which is influenced by the balance of heat lost by convection to the surroundings, lost by conduction through the dies and created by adiabatic heating (iii) the rheological flow, and related defects such as cold shuts and (iv) determining whether excessive grain growth occurs due to the solvus temperature being exceeded, most commonly due to a large contribution from adiabatic heating. The computations represent a rational way of choosing the die geometries and forging sequences, which is of course the primary role of the forgemaster.

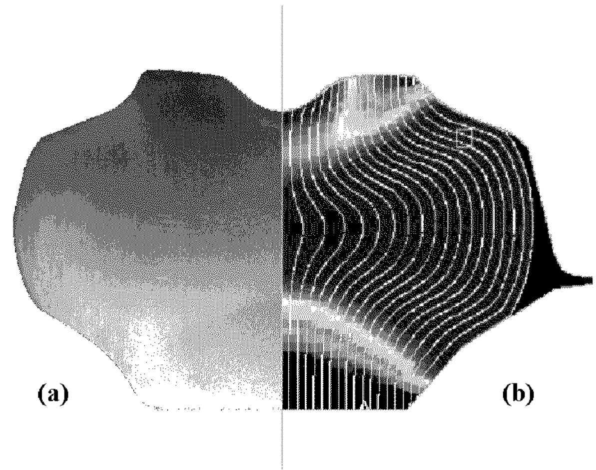

Fig. 7 Closed die forging of INCONEL718 turbine disc. (a) Etched forging illustrating dead zone. (b) Predicted extent of recrystallisation and corresponding flow lines.

After processing, the forgings are subjected to heat treatment followed by a series of machining operations. A number of advantages are conferred by carrying out a thermal elastic-plastic process simulation[8] of this stage of processing, see Fig. 8. These relate to the estimation of the residual stress field, which arises due to the differential thermal contraction of the metal upon cooling, such that the local yield stress is exceeded. Quantification of the stress field allows the subsequent sequence of machining operations to be chosen optimally; problems can otherwise occur due to the relaxation of the stresses as machining proceeds, since

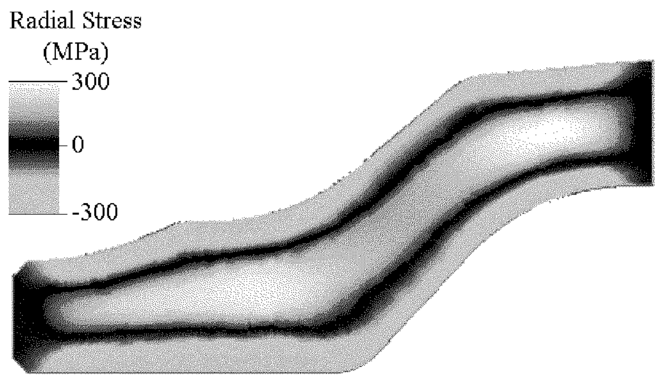

Fig. 8 Predicted radial component of residual stress in an IN718 V2500 aero-engine disc, quenched in oil from 980°C. Cross-section through an axisymmetric finite element mesh of the disc with its axis vertical and centre of symmetry at x=0mm. Regions of high tensile and compressive stress (yellow and blue, respectively), approaching the assumed room temperature yield stress of 300MPa, are clearly visible.

movement of the metal can mean that tolerances can be exceeded. In practice, an accurate estimate of the residual stress field requires an accurate knowledge of the heat transfer between metal and quenching medium; thus heat transfer coefficients must be well characterised. The calculations[8] indicate the plasticity occurs first on the outside surfaces, such that the regions near the free surfaces end up in compression; balancing tensile stresses exist away from the peripheral regions. The stresses are large, and usually a significant fraction of the uniaxial yield stress; the hydrostatic component of the stress field is large too. Recently, we have used neutron diffractometry to confirm the size and extent of the stress field, and so far, the simulations are consistent with the experimental information which has been acquired.

3.4 Simulation of Joining Processes

Joining processes are used widely in the fabrication of turbine engines, particularly for compressor and combustor sections. Often high integrity processes such as electron beam welding (EBW) are employed. The components being assembled are a very long way down the manufacturing stream, so that their value to the turbine manufacturer at this stage is considerable. Thus techniques which help to minimise scrap and non-conformance, e.g. computer modelling and simulation, tend to have great emphasis placed on them. Fortunately, much progress with regard to the analysis of welded structures has been made in recent years. The aim here is to understand and predict the macroscopic transient fields of temperature, displacement, strain and stress, by employing the equations of continuum mechanics. The research[e.g. 9, 10] has reached the point where it is possible to make useful predictions of residual stresses, distortion, cracking and buckling phenomena - the most critical issues from an industrial viewpoint.

The first step is to solve some form of the energy equation, usually with the finite element method; this is because the thermal strain computed from the heat transfer analysis can be considered to provide the driving force for weld-induced distortions. Care must be taken when deciding how to model the heat source, since the physical effects occurring in the molten zone, particularly for processes such as electron beam welding, are not well understood and are subject to debate; thus a balance must be struck between the desire to appeal to all the physical phenomena at play and the practical need to keep the computational cost to within reasonable limits, whilst keeping in mind the numerical answers which need to be generated. The second part of the analysis involves carrying out thermal stress analysis which typically involves large strains and large rotations. The most popular constitutive equation has been elastic-plastic, i.e. creep is not usually accounted for. The basic equations are the conservation of linear momentum, angular momentum, the constitutive equation and the compatibility equation. The chief difficulty arises almost entirely in decomposing the deformation into a translation, rotation and stretch on the one hand and then decomposing the deformation into contributions due to elasticity, plasticity and thermal expansion on the other.

Fig. 9 illustrates a practical example which relates to the electron beam welding of the high pressure compressor assembly of a modern civil aeroengine.[11] This consists of a number of discs which are joined by a weld of length greater than a metre, with secondary (cosmetic) passes added for the purpose of removing weld bead undercut which would otherwise affect the fatigue properties. As a consequence of welding, large residual stresses are set up and these can be estimated for the as-welded state and with an appropriate creep model, after stress-relief heat treatment. The analysis confirms that it is the hoop component of the stress field which is the most significant; thus the weld acts in the same manner as a tourniquet.[11] The transverse (axial) component is smaller, but it is this which is responsible for increasing the separation between the machined disc bores, in

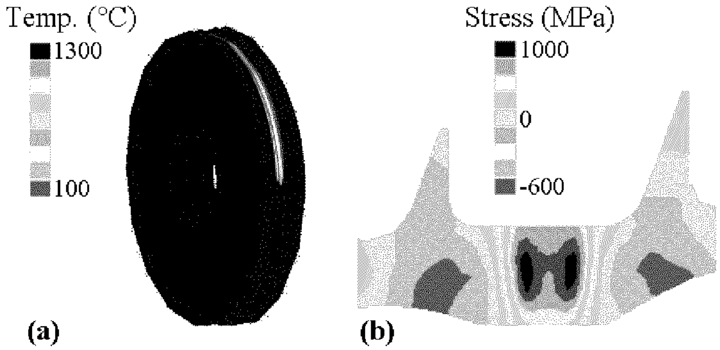

Fig. 9 (a) Predicted thermal field during EB welding of a superalloy compressor assembly. (b) Corresponding residual hoop stress (MPa) after welding.

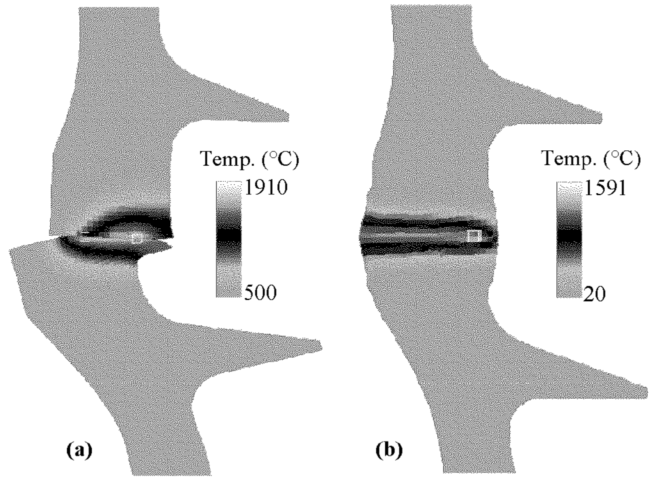

Fig. 10 Simulation of inertia welding of superalloy compressor assembly. (a) Initial jigging arrangement. (b) Modified jigging.

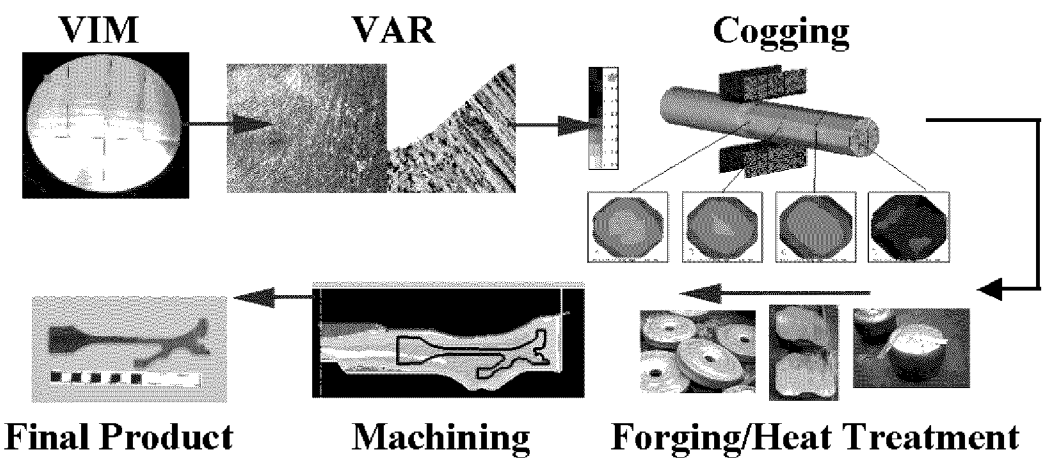

Fig. 11 Digital model of supply chain.

such a manner that the assembly ceases to be exactly radially symmetric; the situation worsens when cosmetic passes are added. The results from these calculations have been compared with measurements made on real assemblies, using needle-probe metrology and neutron diffractometry.[12] These comparisons have convinced us of the power of computer modelling for the anticipation of residual stresses and distortions in welded assemblies such as this. These also provide guidance for the remedial action that needs to be taken when problems arise.

A final example relates to the simulation of the inertia welding of compressor assemblies, see Fig. 10.[13] The temperature capability required of superalloys for hot-end compressor applications is now such that new disc alloys such as RR1000 are being contemplated. Unfortunately, conventional joining processes such as EBW cannot be used since the higher alloying content renders them prone to solidification cracking. Instead, inertia welding must be used. One half of the assembly is accelerated to a significant rotational speed before placing it against the other half, with the aid of an axial load; the heat generated is sufficient to cause a bond without significant melting at the bond. Our calculations indicate that the extent of the bond-line mismatch depends heavily upon the manner in which the two halves of the assembly are held in place during welding; this is consistent with experience.[13] Since the capital cost associated with the jigging arrangement is considerable and it takes up to six months to have it fabricated and delivered, computational modelling has a role to play in the development and application of this joining technology.

4. Summary and Conclusions

In this paper, we have discussed the application of process modelling to support the fabrication of the critical rotating components required for the gas turbine engine. A number of examples have been given. In this field, one aims to build mathematical models of the phenomena occurring during the manufacturing processes. Macroscopic phenomena such as heat flow and continuum mechanics should be included; however, it is becoming increasingly possible to include simulations of microstructure evolution using sophisticated metallurgical models. The emphasis should always be to include as much as possible of the underlying theory, without making the simulations unwieldy, intractable or lengthy. Usually it is necessary to avoid losing sight of the reasons for pursuing a modelling approach.

The major advantages of a building a process model include

- considerable predictive capability, provided that the modelling is sufficiently accurate;
- the provision of an ability to study the effects of changes in the process variables (such as withdrawal rate, geometry, quench rate, welding speed) without resorting to experimental trials;
- the possibility of optimising the processing route in order to reduce and even eliminate manufacturing waste;
- during component prototyping, a potential reduction in the number of design/make iterations which prove necessary; and
- the instilling of greater confidence in a process derived from a better understanding of the physical principles at play.

Future challenges relate to the incorporation of better metallurgical models for microstructure evolution, e.g. solidification, grain growth and texture, which will enable an improved coupling of phenomena occurring on the macro- and micro- scales. Furthermore, more development needs to be carried out to link together the models of the different processes (e.g. casting, forging, heat treatment, welding); this will facilitate the storing of information that characterises the risk of defects being present. We envisage a digital model of the supply chain, see Fig. 11, which allows the appropriate information to be stored, operated upon, and retrieved at various points along the manufacturing route.

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References

1. Zhang, W., Lee, P. D. and McLean, M., *Metall. Mater. Trans. B,* 2002-accepted for publication.
2. Zhang, W., Lee, P. D. and McLean, M., Intermetallics and Superalloys: EUROMAT 99 - Volume 10, D. G. Morris, S. Naka, P. Caron, Eds. (Wiley-Vch, 2000), 123.
3. Xu, X., Zhang, W., Lee, P. D., McLean, M., Ward, R. M. and Jacobs, M. H., Proceedings of Mod. Castings, Welding Adv. Solid. Processes-IX, P. R. Sahm, P. N. Hansen, J. G. Conley, Eds., Aachen, Germany (SHAKER, 2000), 574.
4. Carter, P., Cox, D. C., Gandin, C. A. and Reed, R. C., *Materials Science and Engineering A,* 2000, **280**, 233.
5. Wagner, A., D'Souza, N., Shollock, B. A. and McLean, M., Proc. Int. Sym. on Liq. Metal Proc. & Casting, A. Mitchell, J. Van Den Avyle, Eds., Santa Fe, New Mexico, Sept. 23-26 (AVS, N.Y., N.Y., 2001), 301.
6. Roberts, S. M., Walsh, S. A., Lewis, J. P., Evans, R. W. and Reed, R. C., *Materials Science and Engineering,* 2002 accepted for publication.
7. Dandre, C. A., Roberts, S. M., Evans, R. W. and Reed, R. C., *Mater. Sci. Technol.,* 2000, **16**, 14.
8. Rist, M. A. and Reed, R. C., unpublished work, (University of Cambridge, 2002).
9. Dye, D., Hunziker, O., Roberts, S. M. and Reed, R. C., *Metall. Mater. Trans. A-Phys. Metall. Mater. Sci.,* 2001, **32**, 1713.
10. Dye, D., Hunziker, O. and Reed, R. C., *Acta Mater.,* 2001, **49**, 683.
11. Stone, H. J., Roberts, S. M. and Reed, R. C., *Metall. Mater. Trans. A-Phys. Metall. Mater. Sci.,* 2000, **31**, 2261.
12. Stone, H. J., PhD Thesis, University of Cambridge (1999).
13. Roberts, S. M. and Reed, R. C., unpublished work, (University of Cambridge, 2002).

Paper #11
Discussor' name: Prof. Xiao Guo
Author Trepanier
Q: How are the periods between processes simulated, since the microstructure can change during this time as well as during each processing operation?

A: Most of the changes in the microstructure between process steps occurs with relatively slow kinetics and over large scales, and hence relatively coarse meshes and long timesteps can be used, reducing the computational cost of simulating these transitional periods between the main processing operations.

Discussor's name: Prof. Glyn Davies
Author Trepanier

Q: "You showed some excellent examples of multiscale models for the predictions of properties in metallic systems; is there any similar work on polymer composites?"

A: "I am not aware of any groups simulating the complete manufacturing chain for polymer composites, but individual groups are applying multiscale modeling separately to each step in the processing chain, such as the recent work on the multiscale simulation of Resin Transfer Moulding at Imperial College. This work does need to be brought together and extended to the prediction of properties."